

**Geometric approach to non-relativistic Quantum Dynamics of mixed states**Vicent Gimeno<sup>1, a)</sup> and Jose M. Sotoca<sup>2, b)</sup><sup>1)</sup>*Departament de Matemàtiques- Institute of New Imaging Technologies, Universitat Jaume I, Castelló, Spain.*<sup>2)</sup>*Departamento de Lenguajes y Sistemas Informáticos- Institute of New Imaging Technologies, Universitat Jaume I, Castelló, Spain.*

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In this paper we propose a geometrization of the non-relativistic quantum mechanics for mixed states. Our geometric approach makes use of the Uhlmann's principal fibre bundle to describe the space of mixed states, and, as a new tool, to define a dynamic-dependent metric tensor on the principal manifold, such that the projection of the geodesic flow to the base manifold gives the temporal evolution predicted by the von Neumann equation. Using that approach we can describe every conserved quantum observable as a Killing vector field, and provide a geometric proof for the Poincare quantum recurrence in a physical system with finite energy levels.

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## I. INTRODUCTION

The geometrization of physical theories is a successful and challenging area in theoretical physics. The most well known examples are Hamiltonian mechanics based on symplectic geometry, General Relativity based on semi-Riemannian geometry and classical Yang-Mills theory which uses fibre bundles<sup>11</sup>.

Geometric ideas have also found a clear utility in non-relativistic quantum mechanics problems because quantum theory can be formulated in the language of Hamiltonian phase-space dynamics<sup>12</sup>. Hence, the quantum theory has an intrinsic mathematical structure equivalent of Hamiltonian phase-space dynamics. However the underlying phase-space is not the same space of classical mechanics, but the space of quantum mechanics itself, i.e., the *space of pure states* or the *space of mixed states*.

As opposite to what happens in General Relativity or in Gauge Theory where the metric tensor or the connection are related with the physical interaction, the most usual formulation of the geometry of non-relativistic quantum mechanics is not dynamic, in the sense that is insensitive to changes in the Hamiltonian of the system. Under these assumptions, that approach only makes use of the differential structure of the Hilbert space for quantum states and the Fubini-Study metric. See for example the geometric interpretation of Berry's phase<sup>3</sup>.

From a more dynamical point of view, A. Kryukov<sup>16</sup> has stated that the Schrödinger equation<sup>19</sup> for a pure state  $|\alpha_t\rangle$  (Plank's constant is set equal to 1)

$$\frac{d}{dt} |\alpha_t\rangle = -iH |\alpha_t\rangle \quad , \quad (1)$$

can be considered as a geodesic flow in a certain Riemannian manifold with an accurate metric which depends on the Hamiltonian of the system.

The goal of this paper is to generalize the work of Kryukov for mixed states. To this end, we provide an underlying differential manifold to describe mixed states and a dynamic-dependent Riemannian metric tensor to analyze their temporal evolution.

The mixed states are characterized by density matrices and the equation which plays the role of the Schrödinger one is the von Neumann equation<sup>23</sup>

$$\frac{d\rho_t}{dt} = -i [H, \rho_t] \quad . \quad (2)$$

To obtain the underlying differential manifold, following the Uhlmann's geometrization for non-relativistic quantum mechanics<sup>26–29</sup>, we make use of a principal fibre bundle such that the base manifold of that principal bundle is the space of mixed states. Finally, to provide the Riemannian metric we choose an appropriate metric in the principal bundle, in such a way that the projection of the geodesic flow in the principal manifold to the base manifold is just the temporal evolution given by the von Neumann equation.

Among the geometric properties that are observed due to the movement of this geodesic flow, we analyze in this paper the phase volume conservation according to the Liouville Theorem. That allow us to show a geometric proof of the Poincare recurrence theorem relating it with the recurrence principle for physical systems with discrete energy levels. Let us emphasize that our geometric proof for the quantum Poincare recurrence is closer to the proof for classical mechanics<sup>1</sup> (that also uses the conservation of the volume in the phase-space evolution) than the previous given in the quantum setting<sup>5,22,24</sup>.

## II. DENSITY MATRICES SPACE AS A BASE OF A PRINCIPAL FIBRE BUNDLE

The most general state, the so-called *mixed state*, is represented by a *density operator* in the Hilbert space  $\mathcal{H}$ . In this paper we assume always that  $\dim(\mathcal{H}) = n < \infty$ , being  $\mathcal{H}$  a vector space over the complex field ( $\mathcal{H} = \mathbb{C}^n$ ). The density operator  $\rho$  is in fact a *density matrix*. Recall that a density matrix is a complex matrix  $\rho$  that satisfies the following properties:

1.  $\rho$  is a hermitian matrix, i.e, the matrix coincides with its conjugate transpose matrix:  

$$\rho = \rho^\dagger.$$
2.  $\rho$  is positive  $\rho \geq 0$ . It means that any eigenvalue of  $A$  is non-negative.
3.  $\rho$  is normalized by the trace  $\text{tr}(\rho) = 1$ .

Let us denote by  $\mathcal{P}$  the space of mixed quantum states. Note that the space of pure states  $\mathcal{P}(\mathcal{H})$  is just

$$\mathcal{P}(\mathcal{H}) = \{\rho \in \mathcal{P} \mid \rho^2 = \rho\} \quad .$$

Recall that the space of quantum pure states has an elegant interpretation as a  $U(1)$ -fibre bundle  $\mathcal{S}(\mathcal{H}) \rightarrow \mathcal{P}(\mathcal{H})$ . Following Uhlmann<sup>26–29</sup> and Bengson and Chruściński books<sup>3,9</sup>, we

can use a similar argument to that made in the case of quantum pure states. The key idea of Uhlmann's approach is to lift the system density operator  $\rho$ , acting on the Hilbert space  $\mathcal{H}$ , to an extended Hilbert space

$$\mathcal{H}^{\text{ext}} := \mathcal{H} \otimes \mathcal{H} \quad .$$

In quantum information theory<sup>18</sup>, the procedure of extension,  $\mathcal{H} \rightarrow \mathcal{H}^{\text{ext}}$  is known as attaching an ancilla living in  $\mathcal{H}$ . Obviously, the space of squared matrices  $\mathcal{M}_{n,n}(\mathbb{C})$  ( $n$  rows,  $n$  columns) over  $\mathbb{C}$  (that is a  $2n^2$  real dimensional manifold) can be identified with  $\mathcal{H}^{\text{ext}}$

$$\mathcal{M}_{n,n}(\mathbb{C}) \cong \mathcal{H}^{\text{ext}} \quad .$$

As  $\text{tr}(WW^\dagger)$  is a smooth function over the space of squared matrices, by the Regular Level Set Theorem<sup>17</sup>, the set

$$\mathcal{S}_0 := \{W \in \mathcal{M}_{n,n}(\mathbb{C}) : \text{tr}(WW^\dagger) = 1\} \quad , \quad (3)$$

is a smooth manifold of  $\mathcal{M}_{n,n}(\mathbb{C})$ . Actually, it is no hard to see that  $\mathcal{S}_0$  is diffeomorphic to the sphere  $\mathbb{S}^{2n^2-1}$ . If  $\rho$  is a mixed state in  $\mathcal{P}$ , we shall denote an element  $W \in \mathcal{S}_0$  a *purification* of  $\rho$  if

$$\rho = WW^\dagger \quad , \quad (4)$$

therefore, we get the space of density matrices  $\mathcal{P}$  by the projection  $\pi : \mathcal{S}_0 \rightarrow \mathcal{P}$ , where the projection is given by

$$\pi(W) = WW^\dagger \quad . \quad (5)$$

Observe that, if  $u$  is an unitary matrix (i.e,  $uu^\dagger = u^\dagger u = \mathbb{I}_n$ ) then

$$\pi(Wu) = \pi(W) \quad . \quad (6)$$

Moreover, to fix notation recall that the Lie group  $U(n)$  is a *Lie transformation group*<sup>13</sup> acting on  $\mathcal{S}_0$  on the right. In general, a principal fibre bundle<sup>13</sup> will be denoted by  $P(M, G, \pi)$ , being  $P$  the *total space*,  $M$  the *base space*,  $G$  the *structure group* and  $\pi$  the *projection*. For each  $x \in M$ ,  $\pi^{-1}(x)$  is a closed submanifold of  $P$ , called the *fibre* over  $x$ . If  $p$  is a point of  $\pi^{-1}(x)$ , then  $\pi^{-1}(x)$  is the set of points  $\{pa, a \in G\}$ , and is called fibre through  $p$ .

At this point, an important question to answer, is if  $\mathcal{S}_0(\mathcal{P}, U(n), \pi)$  is a principal fibre bundle over the base manifold  $\mathcal{P}$  of density matrices. Unfortunately the answer is no, because

$U(n)$  doesn't act freely on  $\mathcal{S}_0$ . In general,  $Wu = W$  for  $W \in \mathcal{S}_0$  and  $u \in U(n)$  doesn't imply that  $u = \mathbb{I}_n$ , but observe that if  $\det(W) \neq 0$  ( i.e,  $W$  is an invertible matrix )  $U(n)$  would act freely on our space. This is the way that we shall use to describe the space of density matrices. Instead of start with  $\mathcal{M}_{n,n}(\mathbb{C})$ , we start with the subset of invertible matrices. That subset has the differentiable structure of the Lie group  $GL(n, \mathbb{C})$ . Then, we build a submanifold  $\mathcal{S}$  of  $GL(n, \mathbb{C})$  given by

$$\mathcal{S} := \{W \in GL(n, \mathbb{C}) ; \text{tr}(WW^\dagger) = 1\} \quad . \quad (7)$$

Finally, we obtain the base manifold  $\mathcal{P}^+$  using the projection  $\pi : \mathcal{S} \rightarrow \mathcal{P}^+$  given by

$$\pi(W) = WW^\dagger \quad , \quad (8)$$

and therefore,  $\mathcal{S}(\mathcal{P}^+, U(n), \pi)$  becomes a principal fibre bundle. Observe that

$$\mathcal{P}^+ = \{\rho \in \mathcal{P} \mid \rho > 0\} \quad ,$$

contains only strictly positive (or faithful) density operators. But  $\mathcal{P}$  can be recovered from  $\mathcal{P}^+$  by continuity arguments<sup>3</sup>.

In short, we describe the geometry of the density matrices as a base manifold of a principal fibre bundle consisting of a submanifold  $\mathcal{S}$  of the Lie group  $GL(n, \mathbb{C})$  diffeomorphic to the sphere  $\mathbb{S}^{2n^2-1}$  as a total space and the Lie group  $U(n)$  as structure group.

Since  $\mathcal{S}(\mathcal{P}^+, U(n), \pi)$  admits a global section<sup>20</sup>  $\tau : \mathcal{P}^+ \rightarrow \mathcal{S}$

$$\tau(\rho) := \sqrt{\rho} \quad , \quad (9)$$

therefore  $\mathcal{S}(\mathcal{P}^+, U(n), \pi)$  is a trivial bundle from a topological point of view, that means that<sup>3,13</sup>

$$\mathcal{S} = \mathcal{P}^+ \times U(n) \quad . \quad (10)$$

### III. HAMILTONIAN VECTOR FIELD, DYNAMIC RIEMANNIAN METRIC, SHG-QUANTUM FIBRE BUNDLE AND MAIN THEOREM

In this section, we define a Riemannian metric for dynamics systems and we study how this metric acts within the tangent vector space of  $\mathcal{S}$ . We also discuss the relationship that this metric has with other metrics such as the Bures metric or the metric proposed by Kryukov<sup>16</sup>.

### A. Hamiltonian vector field, dynamic metric and its relation with other metrics

In order to provide explicit expressions for tangent vectors to  $\mathcal{S}$  and the metric tensor, we identify the tangent space  $T_W\mathcal{M}_{n,n}(\mathbb{C})$  with  $\mathcal{M}_{n,n}(\mathbb{C})$  itself. In such a way that since our total space  $\mathcal{S}$  is a submanifold of the manifold  $\mathcal{M}_{n,n}(\mathbb{C})$ , where each point  $W \in \mathcal{S}$  is a matrix, and the tangent space  $T_W\mathcal{S}$  to  $\mathcal{S}$  in the point  $W$  is a subspace of the tangent space  $T_W\mathcal{M}_{n,n}(\mathbb{C})$ . We can use a matrix to describe a point  $W \in \mathcal{S}$  and a matrix to describe a tangent vector  $X \in T_W\mathcal{S}$  too.

First of all, note that the Hamiltonian operator  $H$  induces a vector field  $h : \mathcal{S} \rightarrow T\mathcal{S}$  over  $\mathcal{S}$  given by

$$h_W := -iHW \quad , \quad (11)$$

where  $h_W$  denotes the vector field in the point  $W \in \mathcal{S}$ , i.e,  $h_W = h(W)$ . That vector field  $h$  will be denoted as the *Hamiltonian vector field*.

For any point  $W \in \mathcal{S}$ , and any two tangent vectors  $X, Y \in T_W\mathcal{S}$ , we define the *dynamic Riemannian metric*  $g_H(X, Y)$  as

$$g_H(X, Y) := \frac{1}{2}\text{tr}(X^\dagger H^{-2}Y + Y^\dagger H^{-2}X) \quad . \quad (12)$$

It will be denote by  $\nabla^H$  the Levi-Civita connexion (the sole metric torsion free connexion) given by  $g_H$ . In the definition (12) we use  $H^{-2}$  assuming that  $H$  is an invertible matrix, but that in fact makes no restriction on the Hamiltonian of the system because we can set  $H \rightarrow H + \mathbb{I}_n$  without change the underlying physics. Is not hard to see that  $g_H$  defines a positive definite inner product in each tangent space  $T_W\mathcal{S}$ , being therefore  $g_H$  a Riemannian metric.

With that metric tensor  $g_H$  the (sub)manifold  $(\mathcal{S}, g_H)$  becomes a Riemannian manifold. In order to fix the notation we denote  $\{\mathcal{S}(\mathcal{P}^+, U(n), \pi), h, g_H\}$  the *SHg-quantum fibre bundle of dimension  $n$* .

The rest of this section will devote to study the inherited metric in the base manifold (theorem 1) from the the dynamic metric in the principal manifold and its relation between other metrics.

The tangent space  $T_W\mathcal{S}$  at the point  $W \in \mathcal{S}$  can be decomposed in its horizontal  $H_W$

and vertical  $V_W$  subspaces:

$$T_W\mathcal{S} = H_W \oplus V_W \quad .$$

Observe moreover that the vertical subspace  $V_W$  are the vectors tangent to the fibres. So, any vertical vector  $X_V \in T_W\mathcal{S}$  can be written as

$$X_V = W A \quad ,$$

where  $A \in \mathfrak{u}(n)$  (i.e,  $A$  is an antihermitian matrix). Note that our metric  $g_H$  defines a natural connexion as follows: A tangent vector  $X$  at  $W$  is horizontal if it is orthogonal to the fibre passing through  $W$ , i.e., if

$$g_H(X, Y) = 0 \quad ,$$

for all vertical vector  $Y$  at  $W$  ( $Y \in V_W$ ). Hence  $X \in T_W\mathcal{S}$  is horizontal if

$$X^\dagger H^{-2} W - W^\dagger H^{-2} X = 0 \quad . \tag{13}$$

Therefore, we can define a metric  $g_H^{\mathcal{P}^+}$  in the base manifold at any point  $\rho \in \mathcal{P}^+$ , given by

$$g_H^{\mathcal{P}^+}(Y, Z) := g_H(Y_{\text{Hor}}, Z_{\text{Hor}}) \quad ,$$

where  $Y, Z \in T_\rho\mathcal{P}^+$  and  $Y_{\text{Hor}}$  (respectively  $Z_{\text{Hor}}$ ) is the horizontal lift of  $Y$  (respectively  $Z$ ).

**Theorem 1.** *The metric  $g_H^{\mathcal{P}^+}$  in the base manifold at any point  $\rho \in \mathcal{P}^+$  can be obtained as*

$$g_H^{\mathcal{P}^+}(Y, Z) := \frac{1}{2} \text{tr}(H^{-1} G_Y H^{-1} Z) \quad ,$$

where  $G_Y$  is the unique hermitian matrix satisfying

$$H^{-1} Y H^{-1} = G_Y H^{-1} \rho H^{-1} + H^{-1} \rho H^{-1} G_Y \quad .$$

Note that matrix  $G_Y$  exists and is unique by the existence and uniqueness of the solution of the Sylvester equation<sup>2,25</sup>. Observe moreover that when  $H$  is the identity matrix

$$g_H^{\mathcal{P}^+}(Y, Z) := \frac{1}{2} \text{tr}(G_Y Z) \quad ,$$

where  $G_Y$  is the (unique) solution of

$$Y = G_Y \rho + \rho G_Y \quad ,$$

and that is the Bures metric<sup>10</sup>.

*Proof.* Let  $W : \mathbb{R} \rightarrow \mathcal{S}$  be a curve, such that  $\dot{W}$  is an horizontal vector, then

$$(\dot{W})^\dagger H^{-2} W = W^\dagger H^{-2} \dot{W} \quad .$$

Note, let us define  $A = H^{-1}W$  so

$$\dot{A}^\dagger A = A^\dagger \dot{A} \quad .$$

It is easy to see that the latter condition is fulfilled if

$$\dot{A} = GA \quad , \tag{14}$$

where  $G$  is an Hermitian matrix. Therefore

$$\dot{W} = HGH^{-1}W \quad .$$

Hence applying equation 4

$$\pi_*(\dot{W}) = \dot{W}W^\dagger + W\dot{W}^\dagger = HGH^{-1}\rho + \rho H^{-1}GH \quad . \tag{15}$$

Suppose that

$$\begin{aligned} \pi_*(\dot{W}) &= Y \quad \pi_*(\dot{V}) = Z \\ W(0)W(0)^\dagger &= V(0)V(0)^\dagger = \rho \quad , \end{aligned}$$

then

$$\begin{aligned} g_H^{\mathcal{P}^+}(Y, Z) &= g_H(\dot{W}, \dot{V}) = \frac{1}{2} \text{tr}(\dot{W}^\dagger H^{-2} \dot{V} + \dot{V}^\dagger H^{-2} \dot{W}) \\ &= \frac{1}{2} \text{tr}(H^{-1}G_Y G_Z H^{-1}\rho + H^{-1}G_Z G_Y H^{-1}\rho) \quad , \end{aligned} \tag{16}$$

where

$$\dot{W} = HG_Y H^{-1}W \quad \dot{V} = HG_Z H^{-1}V \quad .$$

Applying equation (15) in  $\pi_*(\dot{V})$

$$Z = HG_Z H^{-1}\rho + \rho H^{-1}G_Z H \quad .$$

Using the above expression (16) the theorem follows.  $\square$

In the case of pure states, our Hilbert space is  $\mathbb{C}^n$  and the tangent space will be  $\mathbb{C}^n$  too. Following Kryukov<sup>16</sup>, we can define a metric  $g_K(X, Y)$  for any two tangent vectors  $X = (x, x^*)$ ,  $Y = (y, y^*)$ , by

$$g_K(X, Y) := \text{Re}(\langle H^{-1}X, H^{-1}Y \rangle) \quad ,$$

where  $\langle X, Y \rangle = \sum_{i=1}^n x_i y_i^*$ , therefore

$$g_K(X, Y) := \frac{1}{2} (\langle H^{-1}X, H^{-1}Y \rangle + \langle H^{-1}Y, H^{-1}X \rangle) = \frac{1}{2} \text{tr}(X^\dagger H^{-2}Y + Y^\dagger H^{-2}X) \quad .$$

When  $H$  is the identity, we recover the Fubini-Study metric.



## B. Geometric structure of the SHg-quantum fibre bundle

As we have seen in the previous sections in the SHg-quantum fibre bundle  $\{\mathcal{S}(\mathcal{P}^+, U(n), \pi), h, g_H\}$  of dimension  $n$ ,  $\mathcal{S}(\mathcal{P}^+, U(n), \pi)$  is a principal (and trivial) fibre bundle,  $\mathcal{S}$  is diffeomorphic to the sphere of dimension  $2n^2 - 1$ ,  $h$  is a vector field on  $\mathcal{S}$ , and  $(\mathcal{S}, g_H)$  is a Riemannian manifold. But the SHg-quantum fibre bundle has more geometric properties :

**Theorem 2** (Main theorem). *Let  $\{\mathcal{S}(\mathcal{P}^+, U(n), \pi), h, g_H\}$  be a SHg-quantum fibre bundle of dimension  $n$ . Then:*

1.  *$h$  is a Killing vector field of  $(\mathcal{S}, g_H)$ .*
2. *The integral curves  $\gamma : I \subset \mathbb{R} \rightarrow \mathcal{S}$  of  $h$  are geodesics of  $(\mathcal{S}, g_H)$ .*
3. *The projection on the base manifold  $\mathcal{P}^+$  of the geodesic  $\gamma$  satisfies the von Neumann equation*

$$\frac{d}{dt}\pi \circ \gamma = -i[H, \pi \circ \gamma] \quad . \quad (17)$$

*Proof.* Condition (1): In order to proof that  $h$  is a Killing vector field, we only have to show that the flow  $\varphi_t : \mathcal{S} \rightarrow \mathcal{S}$  given by

$$\begin{cases} \varphi_0(W) = W, \text{ where } W \in \mathcal{S} \\ \left. \frac{d}{dt}\varphi_t(W) \right|_{t=0} = h_W \quad , \end{cases} \quad (18)$$

is an isometry, i.e, for any  $X, Y \in T_W \mathcal{S}$

$$g_H(\varphi_{t*}(X), \varphi_{t*}(Y)) = g_H(X, Y) \quad . \quad (19)$$

Note that

$$\varphi_{t*}(X) = e^{-iHt} X \quad , \quad (20)$$

and

$$\begin{aligned} g_H(\varphi_{t*}(X), \varphi_{t*}(Y)) &= g_H(e^{-iHt} X, e^{-iHt} Y) \\ &= \frac{1}{2} \text{tr} \left( (e^{-iHt} X)^\dagger H^{-2} e^{-iHt} Y + (e^{-iHt} Y)^\dagger H^{-2} e^{-iHt} X \right) \\ &= \frac{1}{2} \text{tr} \left( X^\dagger e^{iHt} H^{-2} e^{-iHt} Y + Y^\dagger e^{iHt} H^{-2} e^{-iHt} X \right) \\ &= \frac{1}{2} \text{tr} \left( X^\dagger H^{-2} Y + Y^\dagger H^{-2} X \right) = g_H(X, Y) \quad . \end{aligned} \quad (21)$$

Conditions (2) and (3): First of all observe that if  $\gamma$  is the integral curve of the vector field  $h$ , i.e,

$$\dot{\gamma} = h_\gamma = -iH\gamma \quad . \quad (22)$$

The projection of  $\gamma$  satisfies

$$\begin{aligned} \frac{d}{dt}\pi(\gamma(t)) &= \frac{d}{dt}(\gamma(t)\gamma^\dagger(t)) = \dot{\gamma}(t)\gamma^\dagger(t) + \gamma(t)\dot{\gamma}^\dagger(t) = \dot{\gamma}(t)\gamma^\dagger(t) + \gamma(t)(\dot{\gamma}(t))^\dagger \\ &= -iH\gamma\gamma^\dagger(t) + \gamma(t)(-iH\gamma)^\dagger = -i[H, \pi(\gamma(t))] \quad . \end{aligned} \quad (23)$$

Hence, the projection of the integral curves of the vector field  $h$  satisfies the von Neumann equation. So all we have to prove is that curves are actually geodesic curves

$$\nabla_{h_\gamma}^H h_\gamma = 0 \quad . \quad (24)$$

Since  $h$  is a Killing vector field, we only have to proof that  $h$  is an unitary vector field (due any unitary Killing vector field is a geodesic). Namely, the equality

$$\begin{aligned} g_H(h_\gamma, h_\gamma) &= g_H(-iH\gamma, -iH\gamma) = \text{tr}((-iH\gamma)^\dagger H^{-2}(-iH\gamma)) \\ &= \text{tr}(\gamma^\dagger H H^{-2} H \gamma) = \text{tr}(\gamma^\dagger \gamma) = 1 \quad . \end{aligned} \quad (25)$$

Finally, since  $\mathcal{H}$  is an unitary Killing vector field and the integral curves of any Killing vector field of constant length is a geodesic (see appendix theorem 8), the integral curves of  $\mathcal{H}$  are geodesics.  $\square$

**Remark.** Let us emphasize that for any hermitian matrix  $A = A^\dagger$ , we can build the vector field  $\mathcal{A}$  on  $\mathcal{S}$  given by  $-iAW$  for any  $W \in \mathcal{S}$ . It is easy to check in a similar way to equation 21 that if  $[H, A] = 0$ ,  $\mathcal{A}$  is a Killing vector field. Therefore, the set of operators compatibles with the Hamiltonian are related to the set of isometries of  $(\mathcal{S}, g_H)$ , and we can identify any conserved quantum observable with a Killing vector field.

#### IV. GEOMETRIC APPROACH TO QUANTUM POINCARÉ RECURRENCE

As we know from the main theorem,  $h$  is a Killing vector field on the principal manifold  $(\mathcal{S}, g_H)$  endowed with the dynamic metric  $g_H$ . Then, the transformations given by the

1-parametric subgroup  $\varphi_t : S \rightarrow S$  of integral curves of  $h$  are distance-preserving and volume-preserving (see appendix theorem 9). That two facts directly have the following consequences

**Theorem 3** (Insensitivity to Initial Conditions Theorem). *Let  $\{\mathcal{S}(\mathcal{P}^+, U(n), \pi), h, g_H\}$  be a SHg-quantum principal bundle of dimension  $n$ . Then, for any two points  $W, V \in \mathcal{S}$*

$$\text{dist}(\varphi_t(W), \varphi_t(V)) = \text{dist}(W, V) \quad , \quad (26)$$

being the  $\varphi_t$  the 1-parametric subgroup of transformations given by the integral curves of the Killing field  $h$ .

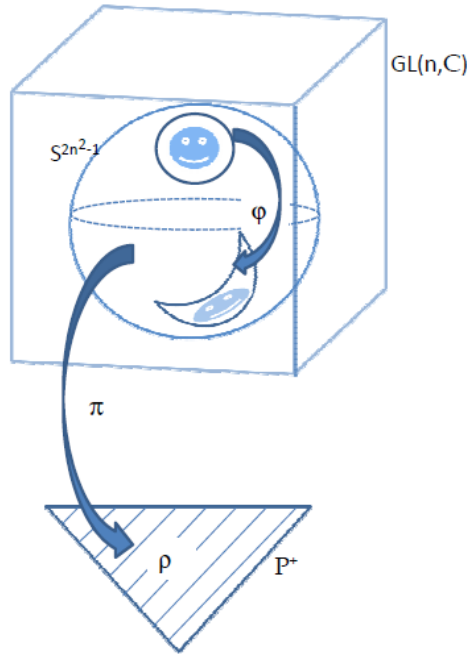


Figure 1. Since the Hamiltonian vector field is a Killing vector field, its flow  $\varphi$  preserves the volume (Liouville theorem) in the sphere  $\mathcal{S}$ , where each point can be projected into the space of density matrices  $\mathcal{P}^+$ .

The classical Liouville theorem<sup>1</sup> states that the natural volume form on a symplectic manifold is invariant under the Hamiltonian flows. In our case, we have the 1-parametric subgroup of transformations  $\varphi_t : \mathcal{S} \rightarrow \mathcal{S}$  given by the integral curves of the Killing field  $h$  and we can set

**Theorem 4** (Liouville Type Theorem). *Let  $\{\mathcal{P}^+, U(n), \pi), h, g_H\}$  be a SHg-quantum principal bundle of dimension  $n$ . Then for any domain  $\Omega \subset \mathcal{S}$*

$$\text{Vol}(\varphi_t(\Omega)) = \text{Vol}(\Omega) \quad , \quad (27)$$

*being the  $\varphi_t$  the 1-parametric subgroup of transformations given by the integral curves of the Killing field  $h$ .*

Using the above theorem, we can therefore state a similar theorem to the Poincare recurrence theorem<sup>1</sup>.

**Theorem 5** (Poincare Type Theorem). *Let  $\{\mathcal{S}(\mathcal{P}^+, U(n), \pi), h, g_H\}$  be a SHg-quantum principal bundle of dimension  $n$ . For any domain  $\Omega \subset \mathcal{S}$  and any time period  $T \in \mathbb{R}^+$  there exist a point  $x \in \Omega$  and a positive integer  $k > 0$  such that*

$$\varphi_{kT}(x) \in \Omega \quad , \quad (28)$$

*being  $\varphi_t : \mathcal{S} \rightarrow \mathcal{S}$  the 1-parametric subgroup of transformations given by the integral curves of the Killing field  $h$ .*

*Proof.* Consider the following sequence of domains

$$\Omega, \varphi_T(\Omega), \varphi_{2T}(\Omega), \dots, \varphi_{kT}(\Omega), \dots$$

All domain in the sequence belongs to the same volume  $\text{Vol}(\Omega)$ . If the above domains never intersect  $\mathcal{S}$  would obtain an infinite volume, but  $\mathcal{S}$  is compact, so  $\text{Vol}(\mathcal{S}) < \infty$ . Then, there exist  $l \geq 0$  and  $m > l$  such that

$$\varphi_{lT}(\Omega) \cap \varphi_{mT}(\Omega) \neq \emptyset \quad , \quad (29)$$

so

$$\Omega \cap \varphi_{(m-l)T}(\Omega) \neq \emptyset \quad . \quad (30)$$

Setting  $k = m - l$  the theorem is proven.  $\square$

Joining the above theorem with the Insensitivity to the Initial Conditions we get

**Theorem 6** (Strong Poincare Type Theorem). *Let  $\{\mathcal{S}(\mathcal{P}^+, U(n), \pi), h, g_H\}$  be a SHg-quantum principal bundle of dimension  $n$ . Then, for any point  $W \in \mathcal{S}$ , any  $\epsilon > 0$  and any  $T \in \mathbb{R}^+$ , there exist a positive integer  $k > 0$  such that*

$$\text{dist}(W, \varphi_{kT}(W)) < \epsilon \quad , \quad (31)$$

being  $\varphi_t : \mathcal{S} \rightarrow \mathcal{S}$  the 1-parametric subgroup of transformations given by the integral curves of the Killing field  $h$ .

*Proof.* Let us consider the domain

$$B_{\frac{\epsilon}{2}}(W) = \left\{ V \in \mathcal{S} : \text{dist}(W, V) < \frac{\epsilon}{2} \right\} . \quad (32)$$

Applying now the Poincare type theorem there must exist  $W_0 \in B_{\frac{\epsilon}{2}}(W)$  and  $k > 0$  such that

$$\varphi_{kT}(W_0) \in B_{\frac{\epsilon}{2}}(W) . \quad (33)$$

So,

$$\text{dist}(W, \varphi_{kT}(W_0)) < \frac{\epsilon}{2} . \quad (34)$$

But, by the Insensitivity to Initial Conditions Theorem

$$\text{dist}(\varphi_{kT}(W), \varphi_{kT}(W_0)) = \text{dist}(W, W_0) < \frac{\epsilon}{2} . \quad (35)$$

Therefore, applying the triangular inequality

$$\text{dist}(W, \varphi_{kT}(W)) \leq \text{dist}(W, \varphi_{kT}(W_0)) + \text{dist}(\varphi_{kT}(W_0), \varphi_{kT}(W)) < \epsilon . \quad (36)$$

□

## A. Physical systems with discrete energy eigenvalues

Using previously stated theorems we can give an alternative proof and more geometric sense of well-known<sup>5,22,24</sup> principle of recurrence for physical systems with discrete energy eigenvalues.

Thus, defining the length  $\|A\|$  of a matrix  $A$  as follows<sup>22</sup>

$$\|A\| = \sqrt{\text{tr}(A^\dagger A)} .$$

Then

**Theorem 7.** *Let  $\rho$  be a mixed state of a quantum system with discrete energy spectrum. Then,  $\rho$  is almost periodic. Namely, for an arbitrarily small positive error  $\epsilon$  the inequality*

$$\|\rho(t+T) - \rho(t)\| < \epsilon \text{ for all } t \quad (37)$$

is satisfied by infinitely many values of  $T$ , these values being spread over the whole range  $-\infty$  to  $\infty$  so as not to leave arbitrarily long empty intervals.

*Proof.* Let  $\rho(t)$  be the density matrix of a system with a discrete set of stationary states, labeled  $n = 0, 1, 2, \dots$ , with energies  $E_n$ , some of which may be equal if there are degeneracies. In energy representation the matrix elements are

$$\rho_{nn'}(t) = \langle n | \rho(t) | n' \rangle \quad . \quad (38)$$

Let  $T_n = |n\rangle\langle n|$  be the projection operator onto the  $n$ th stationary state, then

$$\rho^{nn'}(t) = T_n \rho(t) T_{n'} \quad , \quad (39)$$

is the matrix which in energy representation has only one nonzero element, equal to  $\rho_{nn'}(t)$  and in the location  $(n, n')$ . These matrices are orthogonal in density space

$$\left( \rho^{nn'}(t), \rho^{n''n'''}(t) \right) = \delta_{nn''} \delta_{n'n'''} |\rho_{nn'}(t)|^2 \quad , \quad (40)$$

and

$$\begin{aligned} \rho(t) &= \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \rho^{nn'}(t) \\ &= \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \rho^{nn'}(0) e^{i\omega_{nn'}t} \quad , \end{aligned} \quad (41)$$

where  $\omega_{nn'} = (E_{n'} - E_n)$ . Now, consider the finite sum

$$\sigma^{NN'}(t) = \sum_{n=0}^N \sum_{n'=0}^{N'} \rho^{nn'}(t) \quad (42)$$

as an approximation to  $\rho(t)$ . The square of the error is

$$\begin{aligned} \|\rho(t) - \sigma^{NN'}(t)\|^2 &= \left\| \sum_{n=N+1}^{\infty} \sum_{n'=N'+1}^{\infty} \rho^{nn'}(t) \right\|^2 \\ &= \sum_{n=N+1}^{\infty} \sum_{n'=N'+1}^{\infty} \|\rho^{nn'}(t)\|^2 \\ &= \sum_{n=N+1}^{\infty} \sum_{n'=N'+1}^{\infty} \|\rho^{nn'}(0)\|^2 \end{aligned} \quad (43)$$

The second equality follows from the orthogonality of the  $\rho^{nn'}$ . Since the error is independent of the time,  $\sigma^{NN'}(t)$  converges uniformly to  $\rho(t)$  (in the  $\|\cdot\|$ -norm sense). So  $\rho(t)$  can

be approximate by  $\sigma^{NN'}(t)$ . Since  $\sigma^{NN'}(t)$  is a discrete density with finite energy levels,  $\sigma^{NN'}(t) \in \mathcal{P}^+$ , and the set

$$B_\epsilon^{\mathcal{P}^+}(\sigma^{NN'}(t)) := \{\rho \in \mathcal{P}^+ : \|\rho - \sigma^{NN'}(t)\| < \epsilon\} \quad , \quad (44)$$

is an open precompact set in  $\mathcal{P}^+$ . Using the global section given in equation (9),  $\tau(B_\epsilon)$  will be an open precompact set of  $\mathcal{S}$ . But applying the Strong Poincare Type Theorem for any time period  $T > 0$  there exists  $k > 0$  such that

$$\text{dist} \left( \tau(\sigma^{NN'}(t)), \varphi_{kT}(\tau(\sigma^{NN'}(t))) \right) = \text{dist} \left( \tau(\sigma^{NN'}(t)), \tau(\sigma^{NN'}(t + kT)) \right) < \varepsilon \quad , \quad (45)$$

for any  $\varepsilon > 0$ . Namely,

$$\tau(\sigma^{NN'}(t + kT)) \in B_\varepsilon^{\mathcal{S}}(\tau(\sigma^{NN'}(t))) \quad , \quad (46)$$

being  $B_\varepsilon^{\mathcal{S}}(\tau(\sigma^{NN'}(t)))$  the geodesic ball in  $\mathcal{S}$  centered at  $\tau(\sigma^{NN'}(t))$  of radius  $\varepsilon$ . Now choosing  $\varepsilon$  small enough

$$B_\varepsilon^{\mathcal{S}}(\tau(\sigma^{NN'}(t))) \subset \tau(B_\epsilon^{\mathcal{P}^+}(\sigma^{NN'}(t))) \quad . \quad (47)$$

Therefore by (46)

$$\tau(\sigma^{NN'}(t + kT)) \in \tau(B_\epsilon^{\mathcal{P}^+}(\sigma^{NN'}(t))) \quad . \quad (48)$$

Projecting to the base manifold

$$\sigma^{NN'}(t + kT) \in B_\epsilon^{\mathcal{P}^+}(\sigma^{NN'}(t)) \quad . \quad (49)$$

And, by definition of  $B_\epsilon^{\mathcal{P}^+}(\sigma^{NN'}(t))$

$$\|\sigma^{NN'}(t + kT) - \sigma^{NN'}(t)\| < \epsilon \quad . \quad (50)$$

And the theorem is proven.  $\square$

## V. APPENDIX

In this section we recall several well known results about Killing fields on Riemannian manifolds, for a more detailed approximation see<sup>21</sup>

**Theorem 8.** (see also<sup>4</sup>) Any integral curve  $\gamma : I \subset \mathbb{R} \rightarrow M$  of a Killing vector field  $X$  of constant length  $\sqrt{g(X, X)}$  is a geodesic on  $(M, g)$ .

*Proof.* Here, we need

$$\nabla_{\dot{\gamma}}\dot{\gamma} = \nabla_X X = 0 \quad (51)$$

but, since  $X$  is a Killing vector field the Lie derivative of the metric is zero  $L_X g = 0$  and (see<sup>21</sup> proposition 25)  $\nabla X$  is skew-adjoint relative to  $g$ , so

$$g(\nabla_X X, W) + g(\nabla_W X, X) = 0 \quad (52)$$

for any  $X \in T\mathcal{S}$ . So

$$0 = g(\nabla_X X, W) + 1/2 W(g(X, X)) = g(\nabla_X X, W) \quad (53)$$

then  $\nabla_X X = 0$ . □

**Theorem 9.** *Let  $(M, g)$  be a Riemannian manifold, let  $X$  be a Killing vector field over  $M$ , and denote by  $\varphi_t : M \rightarrow M$  the 1-parametric subgroup of transformations given by  $X$  (i.e.,  $\varphi_0(p) = p$ ,  $\frac{d}{dt}\varphi_t(p)|_{t=0} = X_p$ ), then*

1. *Given any two points  $p, q \in M$ ,  $\text{dist}(p, q) = \text{dist}(\varphi_t(p), \varphi_t(q))$  ,*
2. *Given any domain  $\Omega \subset M$ ,  $\text{Vol}(\varphi_t(\Omega)) = \text{Vol}(\Omega)$ .*

*Proof.* Let  $\varphi_t(\Omega)$  be the flow of the domain  $\Omega$ . Allow us denote

$$V(t) := \text{Vol}(\varphi_t(\Omega)) \quad . \quad (54)$$

Then, the divergence is just (see<sup>8</sup>)

$$V'(0) = \int_{\Omega} \text{div } \mathcal{H} d\mu_{g_H} \quad , \quad (55)$$

where  $d\mu_{g_H}$  denotes the Riemannian density measure.

The divergence is define as<sup>6</sup>

$$\text{div } \mathcal{H} = \text{tr}(Y \rightarrow \nabla_Y^H X) \quad . \quad (56)$$

Given an orthonormal base  $\{E_i\}_{i=1}^{2n^2-1}$  in  $T_W\mathcal{S}$

$$\nabla_Y^H \mathcal{H} = \sum_i Y^i \nabla_{E_i}^H \mathcal{H} = \sum_{i,j} Y^i g_H(\nabla_{E_i}^H \mathcal{H}, E_j) E_j \quad , \quad (57)$$



where  $Y^i := g_H(Y, E_i)$ . Therefore

$$\operatorname{div} \mathcal{H} = \sum_i g_H(\nabla_{E_i}^H \mathcal{H}, E_i) \quad , \quad (58)$$

But since  $\mathcal{H}$  is a Killing field  $\nabla^H \mathcal{H}$  is skew-adjoint relative to  $g_H$  (see<sup>21</sup> proposition 25 again), so

$$\operatorname{div} \mathcal{H} = 0 \quad . \quad (59)$$

And the theorem is proven. □

## REFERENCES

- <sup>1</sup>V. I. Arnol'd, *Mathematical methods of classical mechanics*, Graduate Texts in Mathematics, Vol. 60 (Springer-Verlag, New York, 199?) pp. xvi+516, translated from the 1974 Russian original by K. Vogtmann and A. Weinstein, Corrected reprint of the second (1989) edition.
- <sup>2</sup>R. H. Bartels and G. W. Stewart, “Solution of the matrix equation  $AX + XB = C$ ,” *Comm. ACM* **15**, 820–826 (1972).
- <sup>3</sup>Ingemar Bengtsson and Karol Życzkowski, *Geometry of quantum states* (Cambridge University Press, Cambridge, 2006) pp. xii+466, an introduction to quantum entanglement.
- <sup>4</sup>V. N. Berestovskii and Yu. G. Nikonorov, “Killing vector fields of constant length on Riemannian manifolds,” *Sibirsk. Mat. Zh.* **49**, 497–514 (2008).
- <sup>5</sup>P. Bocchieri and A. Loinger, “Quantum recurrence theorem,” *Phys. Rev. (2)* **107**, 337–338 (1957).
- <sup>6</sup>Manfredo Perdigão do Carmo, *Riemannian geometry*, Mathematics: Theory & Applications (Birkhäuser Boston Inc., Boston, MA, 1992) pp. xiv+300, translated from the second Portuguese edition by Francis Flaherty.
- <sup>7</sup>Isaac Chavel, *Eigenvalues in Riemannian geometry*, Pure and Applied Mathematics, Vol. 115 (Academic Press Inc., Orlando, FL, 1984) pp. xiv+362, including a chapter by Burton Randol, With an appendix by Jozef Dodziuk.
- <sup>8</sup>Isaac Chavel, *Riemannian geometry—a modern introduction*, Cambridge Tracts in Mathematics, Vol. 108 (Cambridge University Press, Cambridge, 1993) pp. xii+386.

- <sup>9</sup>Dariusz Chruściński and Andrzej Jamiołkowski, *Geometric phases in classical and quantum mechanics*, Progress in Mathematical Physics, Vol. 36 (Birkhäuser Boston Inc., Boston, MA, 2004) pp. xiv+333.
- <sup>10</sup>J. Dittmann, “Explicit formulae for the Bures metric,” J. Phys. A **32**, 2663–2670 (1999).
- <sup>11</sup>Jürgen Jost, *Geometry and physics* (Springer-Verlag, Berlin, 2009) pp. xiv+217.
- <sup>12</sup>T.W.B. Kibble, Geometrization of quantum mechanics, Communications in Mathematical Physics **65**, 189–201 (1979).
- <sup>13</sup>Shoshichi Kobayashi and Katsumi Nomizu, *Foundations of differential geometry. Vol. I*, Wiley Classics Library (John Wiley & Sons Inc., New York, 1996) pp. xii+329, reprint of the 1963 original, A Wiley-Interscience Publication.
- <sup>14</sup>Alexey A. Kryukov, “Linear algebra and differential geometry on abstract Hilbert space,” Int. J. Math. Math. Sci. , 2241–2275 (2005).
- <sup>15</sup>Alexey A. Kryukov, “Quantum mechanics on Hilbert manifolds: the principle of functional relativity,” Found. Phys. **36**, 175–226 (2006).
- <sup>16</sup>Alexey A. Kryukov, “On the measurement problem for a two-level quantum system,” Found. Phys. **37**, 3–39 (2007).
- <sup>17</sup>John M. Lee, *Introduction to smooth manifolds*, Graduate Texts in Mathematics, Vol. 218 (Springer-Verlag, New York, 2003) pp. xviii+628.
- <sup>18</sup>Michael A. Nielsen and Isaac L. Chuang, *Quantum computation and quantum information* (Cambridge University Press, Cambridge, 2000) pp. xxvi+676.
- <sup>19</sup>Observe that in equation 1 and throughtout this paper we use the natural units system ( $\hbar = 1$ ).
- <sup>20</sup>The map  $\tau$  is well defined because a positive operator admits a unique positive square root. It is a section because  $\pi(\tau(\rho)) = (\sqrt{\rho})^2 = \rho$ .
- <sup>21</sup>Barrett O’Neill, *Semi-Riemannian geometry*, Pure and Applied Mathematics, Vol. 103 (Academic Press Inc. [Harcourt Brace Jovanovich Publishers], New York, 1983) pp. xiii+468, with applications to relativity.
- <sup>22</sup>Ian C. Percival, “Almost periodicity and the quantal  $H$  theorem,” J. Mathematical Phys. **2**, 235–239 (1961).
- <sup>23</sup>Jun John Sakurai, *Modern Quantum Mechanics; rev. ed.* (Addison-Wesley, Reading, MA, 1994).
- <sup>24</sup>L. S. Schulman, “Note on the quantum recurrence theorem,” Phys. Rev. A **18**, 2379–2380 (1978).

- <sup>25</sup>J. Sylvester, “Sur l’équation en matrices  $px = xq$ ,” C.R. Acad. Sci. Paris **99**, 67–71 (1884).
- <sup>26</sup>A. Uhlmann, “Parallel transport and holonomy along density operators,” Tech. Rep. (Leipzig Univ., Leipzig, 1987).
- <sup>27</sup>A. Uhlmann, “On Berry phases along mixtures of states,” Ann. Physik (7) **46**, 63–69 (1989).
- <sup>28</sup>Armin Uhlmann, “Parallel transport and “quantum holonomy” along density operators,” Reports on Mathematical Physics **24**, 229 – 240 (1986).
- <sup>29</sup>Armin Uhlmann, “A gauge field governing parallel transport along mixed states,” Lett. Math. Phys. **21**, 229–236 (1991).

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